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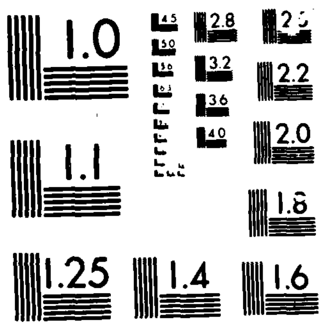

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Light Scattering from a Deep Metallic Grating

by

Dan Agassi and Thomas F. George

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Buffalo, New York 14260

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The conditions under which the Rayleigh hypothesis is exact and the convergence properties of the Rayleigh expansion are considered. The identification of the cause of the deficiency of this expansion suggests an alternative "dressed" expansion with presumably simpler convergence properties. This proposition is checked for a sinusoidal grating (SG), for which convergence is found for an arbitrary value of $\beta = 2\pi g/d$, where g and d denote the height and periodicity of the SG, respectively. The dressed expansion is used to analyze the surface plasmon dispersion and local field enhancement distribution pertaining to the SG in the limit as β goes to infinity. The dispersion relation is comprised of two bands. The local field enhancement predicts stronger fields at the bottoms of the troughs than at the peaks of the SG.

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LIGHT SCATTERING FROM A DEEP METALLIC GRATING

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ABSTRACT

The conditions under which the Rayleigh hypothesis is exact and the convergence properties of the Rayleigh expansion are considered. The identification of the cause of the deficiency of this expansion suggests an alternative "dressed" expansion with presumably simpler convergence properties. This proposition is checked for a sinusoidal grating (SG), for which convergence is found for an arbitrary value of $\beta = 2\pi g/d$, where g and d denote the height and periodicity of the SG, respectively. The dressed expansion is used to analyze the surface plasmon dispersion and local field enhancement distribution pertaining to the SG in the limit as β goes to infinity. The dispersion relation is comprised of two bands. The local field enhancement predicts stronger fields at the bottoms of the troughs than at the peaks of the SG.

INTRODUCTION

Light scattering from a grating is a well-developed subject in classical optics.[1] The underlining, well-known physical process is (elastic) Bragg scattering, i.e., the exchange of surface-parallel momentum between the grating and the incident light by an amount nk_G, where $n = 0, \pm 1, \pm 2, \ldots$ and the grating momentum is $k_G = 2\pi/d$. All notations are defined in Fig. 1. It is, however, important to

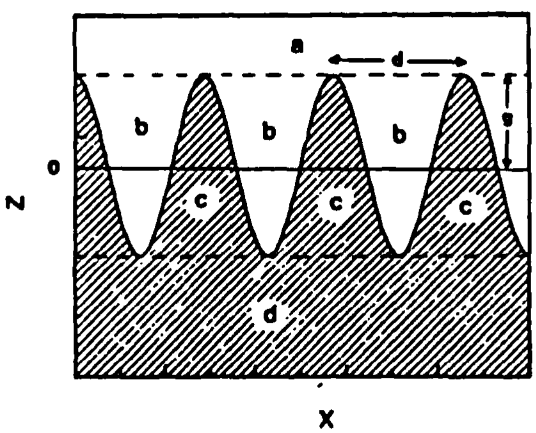

Fig. 1. Generic grating defining the notations. The incident light is directed downward, and the hatched area indicates the metal. The domains "a"-"d" pertain to the discussion of the Rayleigh expansion.

realize that, barring a few recent studies,[2-6] most of the work pertains to the restricted physical domain of shallow gratings where $\beta = 2\pi g/d < 1$. Light scattering from such gratings is

qualitatively different from that pertaining to deep gratings, i.e., when $\beta \gg 1$. In the former case, the grating can exchange only a limited number of k_G quanta, i.e., $n \sim \Theta(1)$. Consequently, the scattered light is comprised of a dominant specular and a few Bragg components. On the other hand, for deep gratings, $n \sim \Theta(\beta) \gg 1$ (see below). Hence, the scattered light is comprised of many, equally important and strongly interfering Bragg components, which gives the scattered light a new qualitative character. The theoretical description of the deep grating domain is at the focus of this paper.[7]

RAYLEIGH EXPANSION AND HYPOTHESIS

The Rayleigh expansion[1,8] provides a framework to the shallow grating work and a starting point to our analysis. It results from the underlying symmetry of the grating: Since it is invariant under translations $x \to x+nd$, where n is any integer, the Floquet-Bloch theorem implies that the electromagnetic field $\vec{\Psi}(x,z)$ has the property $\vec{\Psi}(x+d,z) = \exp[ik_\parallel d]\vec{\Psi}(x,z)$ where $k_\parallel$ is a surface-parallel (Fig. 1) momentum label.[4] Consequently, the Fourier series expansion of the fields in a "unit cell" $0 \leq x \leq d$ (the z-dependence is determined from the wave equation) suffices to describe the field throughout the xz-plane. When the proper boundary conditions at infinity and the vector character are incorporated, the ensuing p-wave expansion is the Rayleigh expansion:

$$\vec{E}_\alpha(x,z) = \sum_{\ell=-\infty}^{\infty} \{C_\alpha(\ell)\hat{p}_{\alpha,-}(\ell)e^{i[k_\ell x - W_\alpha(\ell)z]} + A_\alpha(\ell)\hat{p}_{\alpha,+}(\ell)e^{i[k_\ell x + W_\alpha(\ell)z]}\} , \tag{1}$$

where

$$k(\alpha) = \sqrt{\epsilon_\alpha}k , \qquad k = \omega_0/c , \qquad k_G = 2\pi/d , \qquad \beta = gkG,$$

$$W_\alpha(\ell) = [k^2(\alpha)-k_\ell^2]^{1/2} , \quad k_\ell = k + \ell k_G , \quad \mathrm{Re}(W_d),\mathrm{Im}(W_\sigma) \geq 0,$$

$$\hat{p}_{\alpha,\pm}(\ell) = \frac{1}{k(\alpha)}[k_\ell\hat{z} \mp W_\alpha(\ell)\hat{x}], \qquad \hat{s} = \hat{x} \times \hat{z} \quad . \tag{2}$$

In (2), $\hat{x}$ and $\hat{z}$ are unit vectors in the x- and z- directions (Fig.1), and α denotes a domain in the xz-plane with a constant dielectric constant ϵ_α. Once a convenient partition of the xz-plane into domains has been chosen, the coefficients C_α, A_α are determined by matching the boundary conditions across the domain boundaries. To avoid mathematical pitfalls in the subsequent discussion, we confine ourselves henceforth to gratings such that the fields are non-singular everywhere.

The Rayleigh hypothesis can now be introduced in terms of expansions (1). For example, the grating in Fig. 1 calls for four expansions (1) while the Rayleigh hypothesis asserts that only two

are needed since the expansions in domains "a" and "b" are identical and likewise for domains "c" and "d". By matching the boundary conditions across the ($z=g$)-plane, we conclude that the hypothesis is exact for gratings whose profile is expressible in terms of a finite Fourier series. For other gratings, the Rayleigh hypothesis may, or may not be exact.

DRESSED RAYLEIGH EXPANSION

Attempts to apply the Rayleigh expansion to deep-grating calculations indicate its divergence for $\beta > 0.6$ (sinusoidal gratings).[11] This situation has motivated the introduction of alternative schemes[2-6,12] in the quest to enlarge the β-range accessible for calculations. Our approach is to expose the origin of the instability of (1) when $\beta \gg 1$, which then naturally leads to an alternative expansion -- the dressed expansion -- with excellent convergence properties.[10]

For the grating in Fig. 1, the expansion in domain "0", which combines domains "a" and "b", is

$$\vec{E}_0(x,z) = \vec{E}_{in} + \sum_{\ell=-\infty}^{\infty} A_0(\ell)\hat{p}_{0,+}(\ell)e^{i[k_\ell x + W_0(\ell)z]} , \tag{3}$$

Disregarding the uninteresting phase $\exp(ik_\ell x)$ and geometrical factor $\hat{p}_{0,+}(\ell)$ in (3), the $|\ell| \to \infty$ behavior is (see (2)):

$$A_0(\ell)e^{iW_0(\ell)z} \xrightarrow[|\ell|\to\infty]{} A_0(\ell)e^{-k_G|\ell|z} . \tag{4}$$

Consequently, at the bottom of a trough, where $-g \leq z \leq 0$, the z-dependent factor in (4) diverges exponentially. Therefore, to render the total field $\vec{E}_0(x,z)$ finite, the <u>exact</u> $A_0(\ell)$ must converge at least as $\exp(-\beta|\ell|)$. Hence for $z < 0$,(3) is a sum of energy terms, most of which are products of exponentially large factors times exponentially small numbers. The <u>calculated</u> $A_0(\ell)$, however, always entail an error which, when multiplied by $\exp(\beta|\ell|)$, yields large erros in $\vec{E}_0(x,z)$. Thus, (3) is intrinsically unstable as a scheme for $\beta \gg 1$ (many $|\ell|$'s) calculations.

This deficiency is easily remedied by rewriting (4) as

$$A_0(\ell)e^{iW_0(\ell)z} = \alpha_0(\ell)e^{iW_0(\ell)(z+g)} , \tag{5}$$

where $\alpha_0(\ell) = A_0(\ell)\exp[-iW_0(\ell)z]$. By construction the RHS of (5) always converges for $z+g > 0$, and when $z+g = 0$, the $\alpha_0(\ell)$ converge to render, by assumption, a finite $\vec{E}_0(x,z)$ on the grating's surface. Therefore, by transcribing (1) into the "dressed" expansion, as defined by the transformation (5), a major flaw in (1) is eliminated.

The convergence of the dressed expansion can be explicitly demonstrated for a sinusoidal metallic grating.[10] Lack of space does not allow us to outline the analysis. The results are that the dressed expansion converges for an arbitrary large β, and the number of significant components in the dressed expansion is on the order $N \sim 4\beta$. This analysis also explains why the (bare) Rayleigh expansion diverges for $\beta \gtrsim 0.6$.[11]

SURFACE PLASMON (SP) DISPERSION RELATION IN THE $\beta \to \infty$ LIMIT

As an application of the dressed expansion, we consider the SP dispersion relation[13] in the $\beta \to \infty$ limit for a sinusoidal grating.[13] Lack of space allows us only quote the result:

$$\frac{[3k^2(0) + k^2(1))(k^2(0) + 3k^2(1)]}{3[k^2(0) + k^2(1)]^2}$$

$$= \left\{\frac{\sin[L(\alpha+\gamma)]\sin[\frac{\alpha-\gamma}{2}] - \sin[L(a-\gamma)]\sin[\frac{\alpha+\gamma}{2}]}{\sin[L(\alpha+\gamma)]\sin[\frac{\alpha-\gamma}{2}] + \sin[L(\alpha-\gamma)]\sin[\frac{\alpha+\gamma}{2}]}\right\}^2 , \qquad (6)$$

where $k(i) = k\sqrt{\epsilon_i}$ from Eq. (1), $\gamma = 2\pi k/k_G$,

$$\alpha = \frac{\pi}{k_G}\{-[k^2(0) + k^2(1)]\}^{1/2} , \qquad (7)$$

and $L \sim \Theta(\beta) >> 1$, the precise value of which is immaterial.

The analysis of (6) is straightforward: The LHS is a smooth function of $x = k/k_p$, where $k_p = \omega_p/c$ and ω_p is the (volume) plasmon frequency. At $x = 0$ it is unity, decreasing monotonically to $-\infty$ at $x = 1/\sqrt{2}$ and subsequently increasing and becoming positive for $x \geq \sqrt{3}/2$. The RHS of (6), on the other hand, is rapidly oscillating with frequency $\sim 1/\beta$ and amplitude $\sim \beta$. Furthermore, since α (Eq. (7)) is real for $x < 1/\sqrt{2}$ and imaginary for $x > 1/\sqrt{2}$, the RHS of (6) is positive and negative, respectively. Consequently, (6) has a large number of solutions ($\Theta(\beta)$) in the domains $0 \leq x \leq 1/2$ and $\sqrt{2}/2 \leq x \leq \sqrt{3}/2$.[13] The frequency band gap between these two band is hence $\Delta\omega/\omega_p = (\sqrt{2}-1)/2$. This outcome is in keeping with the known behavior for $\beta << 1$.[14]

In summary, we have exposed the reason for the poor convergence of the Rayleigh expansion when $\beta >> 1$, and introduced an alternative expansion -- the dressed expansion -- which has allegedly very good convergence properties. This premise is explicitly demonstrated for a sinusoidal grating. We have also discussed the surface plasmon dispersion relation in the $\beta \to \infty$ limit, where we find that the branches tend to cluster into two bands separated by $\Delta\omega/\omega_p = (\sqrt{2}-1)/2$.

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